

Quantum fidelity and thermal phase transitions

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We study the quantum fidelity approach to characterize thermal phase transitions. Specifically, we focus on the mixed-state fidelity induced by a perturbation in temperature. We consider the behavior of fidelity in two types of second-order thermal phase transitions (based on the type of nonanalyticity of free energy), and we find that usual fidelity criteria for identifying critical points is more applicable to the case of λ transitions (divergent second derivatives of free energy). Our study also reveals that for fixed perturbations, the sensitivity of fidelity at high temperatures (where thermal fluctuations wash out information about the transition) is reduced. From the connection to thermodynamical quantities we propose slight variations to the usual fidelity approach that allow us to overcome these limitations. In all cases we find that fidelity remains a good precriterion for testing thermal phase transitions, and we use it to analyze the nonzero temperature phase diagram of the Lipkin-Meshkov-Glick model.

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I. INTRODUCTION

Quantum phase transitions (QPTs) [1], the sudden change in the properties of a quantum many-body system as a control parameter is varied, have been the focus of a wealth of research in the past decades. Once almost exclusively the domain of condensed matter physics, the field of quantum critical phenomena has recently attracted the attention of the quantum information community: some quantum entanglement measurements [2] such as concurrence [3], entanglement entropy [4], and geometric phase [5] can exhibit singular behavior at quantum critical points. Thus, they can be used in place of macroscopic thermodynamic quantities in classical statistical mechanics—e.g., specific heat and magnetic susceptibility—not only to characterize different QPTs, but also to gain insight on the nature of the quantum critical behavior.

Motivated by the sensitivity to perturbations of quantum systems near a critical region, one of us and collaborators [6] proposed to use the Loschmidt echo [7] as another quantum information probe of QPTs [8]. Based on this work, Zanardi *et al.* further proposed a geometric measure: the quantum fidelity [9] (the overlap) between two ground states corresponding to slightly different values of the controlling parameters. A flurry of work ensued [10,11], showing that, despite its simplicity, quantum fidelity does indeed capture the dramatic changes in the structure of the ground state at a quantum critical point. In particular, it has been observed that for second order QPTs fidelity presents a minimum at the critical point [9], which became the standard criterion for detecting quantum criticality with fidelity. Though fidelity is used to study QPTs at zero temperature, its finite-temperature (thermal state) extension has also been considered [12]. The motivation behind this approach is similar to that for QPTs: The proximity to criticality must be reflected in the geometric distance between two states separated by a small perturbation (either in temperature or in an external parameter). The fidelity of mixed states [13,14] at finite temperature also gives useful information about the zero-temperature phase diagram [12]. Studies of finite temperature transitions using

this fidelity approach have been reported for specific models, such as the Stoner-Hubbard itinerant electron model of magnetism, the BCS model [15], and also the crossover at finite temperature in the one-dimensional transverse Ising model (TIM) [16]. Nevertheless, we find that, in the existing literature, the mechanism for which fidelity can be used to characterize thermal phase transitions has not been studied systematically. Here, we will study the applicability of the mixed-state fidelity approach to general second-order thermal phase transitions. We will focus on nonzero temperature phase diagrams and illustrate our arguments with specific examples. Finally, we will also discuss the quantum-classical transition of the system when increasing the temperature from a new angle: the relation between quantum fidelity and magnetic susceptibility. In the rest of this work, and unless explicitly stated, we will use the term fidelity to mean mixed-state fidelity.

This paper is organized as follows. In Sec. II, we introduce the finite-temperature mixed-state fidelity and study its relation to the analyticity of free energy. In particular, we show why fidelity can signal phase transitions by establishing its relationship to specific heat and magnetic susceptibility. In Sec. III we study examples of two types of second-order thermal phase transitions—either a divergence or a discontinuity of specific heat at critical points—and discuss the corresponding behavior of mixed-state fidelity. The problems in characterizing the second type of transitions with fidelity will be shown. In Sec. IV we discuss two problems of the fidelity approach to thermal phase transitions, and possible solutions: fidelity decay alone cannot distinguish between phase transitions and crossovers, and at high-temperature thermal fluctuations that can reduce the effectivity of fidelity for picking out critical points. The workaround to these problems will come from the insight gained with the connection of fidelity and standard thermodynamical quantities. In Sec. V, we use the Lipkin-Meshkov-Glick model as an example to demonstrate that, despite its limitations, fidelity remains a useful pre-criteria for thermal phase transitions due to its simple form.

II. FINITE-TEMPERATURE FIDELITY AND ITS RELATION TO SPECIFIC HEAT AND MAGNETIC SUSCEPTIBILITY

The mixed-state fidelity of two thermal states with small perturbations in temperature and controlling parameter is defined as [12–14]

$$\mathcal{F}(\beta_0, \lambda_0; \beta_1, \lambda_1) = \text{Tr} \sqrt{\sqrt{\rho_0} \rho_1 \sqrt{\rho_0}}, \quad (1)$$

where the thermal states are written in terms of the Hamiltonian H of the system

$$\rho_\alpha = \frac{e^{-\beta_\alpha H(\lambda_\alpha)}}{Z(\beta_\alpha, \lambda_\alpha)}, \quad (2)$$

with the partition function

$$Z(\beta_\alpha, \lambda_\alpha) = \text{Tr} e^{-\beta_\alpha H(\lambda_\alpha)}, \quad (3)$$

and where we have perturbations in the Hamiltonian parameter $\lambda_1 = \lambda_0 + \delta\lambda$ and in temperature $\beta_0 = 1/k_B T_0$, $\beta_1 = 1/k_B(T_0 + \delta T)$. In the following we set Boltzmann’s constant k_B to unity. It can be checked that when both temperatures T_0 and T_1 decrease to zero, the mixed-state fidelity reduces to the ground-state fidelity $|\langle \phi_{g.s.}(\lambda) | \phi_{g.s.}(\lambda + \delta\lambda) \rangle|$, where $|\phi_{g.s.}(\lambda)\rangle$ is the ground state of Hamiltonian $H(\lambda)$ for a particular value of the controlling parameter λ .

When $\delta\lambda = 0$, we define the temperature fidelity $\mathcal{F}_\beta(\beta_0, \beta_1, \lambda) \equiv \mathcal{F}(\beta_0, \lambda; \beta_1, \lambda)$, which simplifies to

$$\mathcal{F}_\beta(\beta_0, \beta_1, \lambda) = \frac{Z\left(\frac{\beta_0 + \beta_1}{2}, \lambda\right)}{\sqrt{Z(\beta_0, \lambda)Z(\beta_1, \lambda)}}. \quad (4)$$

It can be further proved (see Appendix A) that for small perturbations $\delta T/T \ll 1$ [18]

$$\mathcal{F}_\beta(\beta_0, \beta_1, \lambda) \approx e^{-[(\delta\beta)^2/8\beta^2]C_v}, \quad (5)$$

where $C_v = -T\partial^2 F/\partial T^2$ is the specific heat at constant field obtained from the free energy F of the system. It is interesting to notice that the temperature fidelity defined in Eq. (4) can be used for a classical system as well as for a quantum system, since it only has partition functions. This surprising applicability, a quantum measure used for classical systems, can be understood in terms of a map that allows to identify any $T > 0$ phase transition in a classical lattice system with a quantum phase transition of a quantum model in the same lattice [17]. In a basis that maps one quantum state $|\sigma\rangle$ to each allowed classical state σ , the associated quantum model has a ground state whose coefficients are the square root of the Boltzmann weight of the corresponding energies, i.e., $|g(\beta)\rangle = \sum_\sigma \exp(-\beta E_\sigma/2)|\sigma\rangle/\sqrt{Z(\beta)}$. The quantum model can be thought of as “quantum simulating” the classical system, whose thermodynamical properties can be found by a proper quantum annealing to the ground state [17]. Therefore, it is straightforward to see that Eq. (4) used for a classical system corresponds to the usual ground-state fidelity (as defined by Zanardi [9]) of the associated quantum simulator evaluated at neighboring temperatures β_0 and β_1 .

When $\delta T = 0$, we can define $\mathcal{F}_\lambda(\beta, \lambda_0, \lambda_1) \equiv \mathcal{F}(\beta, \lambda_0; \beta, \lambda_1)$, which can be approximated as (see Appendix B)

$$\mathcal{F}_\lambda(\beta, \lambda_0, \lambda_1) \approx \frac{Z\left(\beta, \frac{\lambda_0 + \lambda_1}{2}\right)}{\sqrt{Z(\beta, \lambda_0)Z(\beta, \lambda_1)}}. \quad (6)$$

The approximation in Eq. (6) is due to the fact that, in general, $H(\lambda_0)$ and $H(\lambda_1)$ do not commute with each other, and is valid only for high temperatures such that $\beta^3 \delta\lambda^3 \ll 1$. From Eq. (6), and using arguments similar to those used for Eq. (5), it can be shown that [19] (see Appendix C)

$$\mathcal{F}_\lambda(\beta, \lambda_0, \lambda_1) \approx e^{-[\beta(\delta\lambda)^2/8]\chi}, \quad (7)$$

where $\chi = -\partial^2 F/\partial\lambda^2$ is the susceptibility to an external field of strength $\lambda = (\lambda_0 + \lambda_1)/2$.

We see then from Eqs. (5) and (7) how the fidelity criterion for detecting a second-order phase transition [16,18,20] plays out for mixed-state fidelity: The minima of \mathcal{F} are associated with the singularities of the specific heat and magnetic susceptibility. More generally, as we will see below, \mathcal{F} inherits all nonanalyticities of the free energy, be them divergences or discontinuities in its second derivatives. Therefore, it is reasonable to expect that fidelity can be used to study thermal phase transitions, just like traditional criteria based on specific heat or susceptibilities.

It is interesting to note that from the above Eqs. (5) and (7) we can also obtain the so-called perturbation-independent fidelity susceptibilities [18]

$$\chi_\beta \equiv \frac{-2 \ln \mathcal{F}_\beta}{(\delta\beta)^2} \approx \frac{1}{4\beta^2} C_v, \quad (8)$$

$$\chi_\lambda \equiv \frac{-2 \ln \mathcal{F}_\lambda}{(\delta\lambda)^2} \approx \frac{\beta}{4} \chi. \quad (9)$$

We would like to emphasize that Eqs. (6) and (9) hold approximately only for high temperatures, and are a bad approximation for low temperatures and especially for zero temperature, where quantum commutation relations are relevant. We will discuss this point in Sec. IV. Usually the calculation of \mathcal{F}_λ is much more difficult than that of \mathcal{F}_β due to the noncommutativity of $H(\lambda_0)$ and $H(\lambda_1)$. In the following we will focus on the fidelity for a perturbation in temperature \mathcal{F}_β , and its application to second-order thermal phase transitions.

III. FIDELITY IN SECOND-ORDER THERMAL PHASE TRANSITIONS

Second-order thermal phase transitions are characterized by nonanalyticities in second derivatives of the free energy (e.g., specific heat, susceptibility) with respect to thermodynamic variables (temperature and external magnetic fields). According to standard classification [21], there are two types of nonanalyticity that need to be considered: discontinuities and divergences (also known as λ transition). For ordering purposes we call the associated transitions type A and type B,

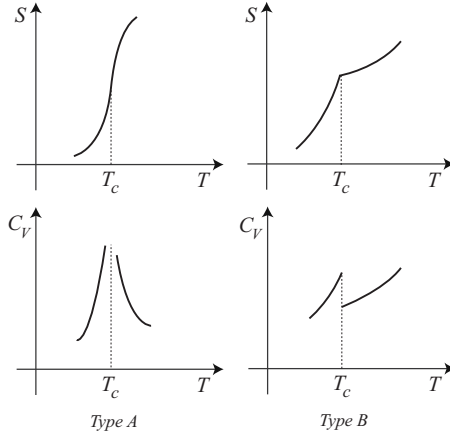


FIG. 1. Schematic diagrams of two types of second order phase transition. Type A corresponds to a divergence of second derivative of free energy, while type B corresponds to a discontinuity (jump) of second derivative of free energy. In this example we plot the first and second derivative of free energy that correspond to entropy and specific heat respectively. Second-order phase transitions of type A are also called λ transitions.

respectively, shown schematically in Fig. 1. In the following we will discuss the behavior of fidelity near the critical points associated to these two types of thermal phase transitions.

A. Type A: divergence of second-order derivative of free energy

In this type of transition—an example of which is the phase transition in the λ line of ^4He —the specific heat at the

critical point is much larger than that at other points, and diverges in the thermodynamic limit. From Eq. (5) we know that the critical point signaled by the maximum C_V will correspond to a minimum of fidelity \mathcal{F} . Thus, for this type of systems the decay of fidelity as a function of the parameters (and with a fixed perturbation δT) can be used to characterize accurately the phase boundaries. A good example of this situation is the two-dimensional (2D) classical Ising model. This system is described by the Hamiltonian $H = -J \sum_{\langle i,j \rangle} s_i s_j + \lambda \sum_i s_i$, where $\langle i,j \rangle$ means sum over nearest-neighbor sites $s_i = \pm 1$ and λ is the external magnetic field. Onsager's famous solution [22] gives the partition function for zero external magnetic field ($\lambda = 0$),

$$Z(\beta, \lambda = 0) = \exp \left\{ N \ln [2 \cosh(2\beta J)] + \frac{N}{2\pi} \int_0^\pi d\phi \ln \left[\frac{1 + \sqrt{1 - K^2 (\sin \phi)^2}}{2} \right] \right\}, \quad (10)$$

where $K = 2 \sinh(2\beta J) / [\cosh(2\beta J)]^2$. By inserting this into Eq. (4), we can obtain the fidelity $\mathcal{F}_\beta(\beta_0, \beta_1, \lambda)|_{\lambda=0}$ for the 2D classical Ising model [see Fig. 2(a) for the case of $\delta T = 0.001$ and $\delta\lambda = 0$].

The minimum of fidelity agrees well with the analytical result for the critical temperature $T_c \approx 2.27J$ (see for comparison the specific heat on the right panel). Since fidelity decays only on the critical lines, we conclude then that its minimum is a good indicator of criticality in this type of transitions. Nevertheless, we would like to point out that the decay of fidelity at the critical points becomes less drastic for higher temperatures for a fixed δT . This is because thermal

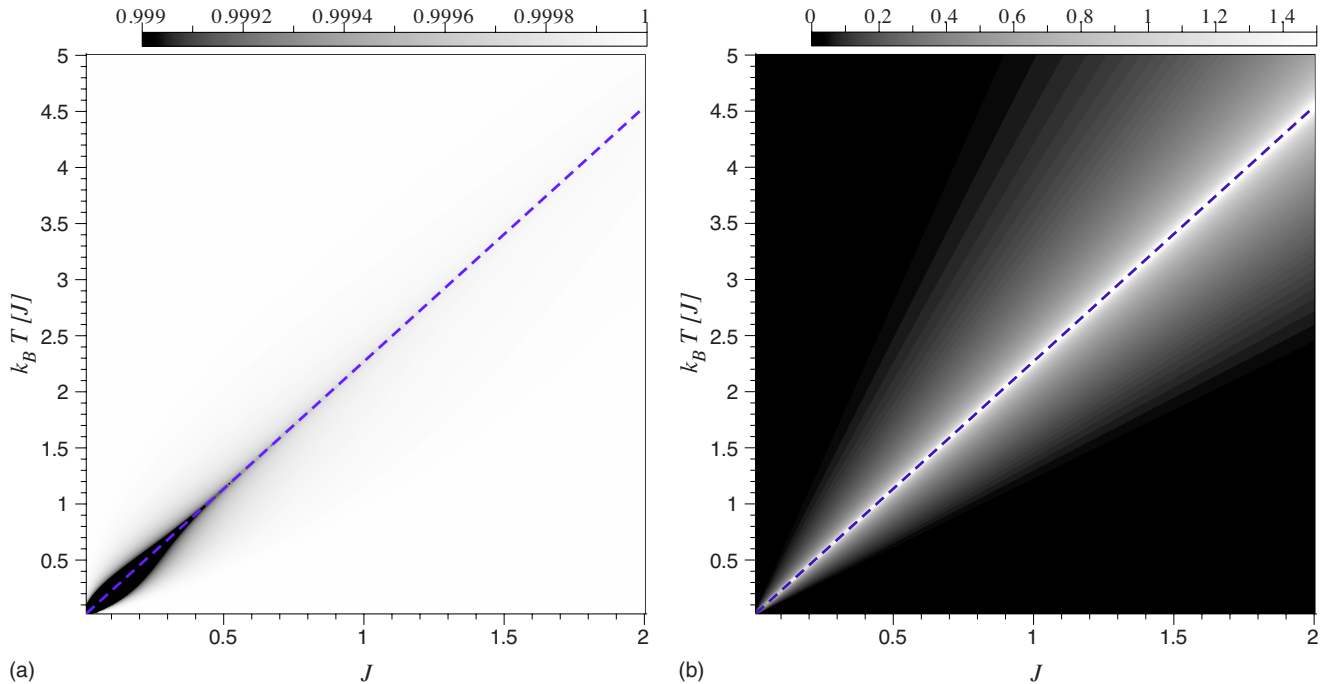


FIG. 2. (Color online) Fidelity (left) and specific heat (right) of the 2D Ising model at zero external field and $N=2000$, $\delta T=0.001$. The critical temperature $T_c \approx 2.27J$, indicated by the dashed line, is clearly signaled by the minimum of fidelity. Because the specific heat diverges at the critical point, the 2D Ising model corresponds to a type-A second-order phase transition.

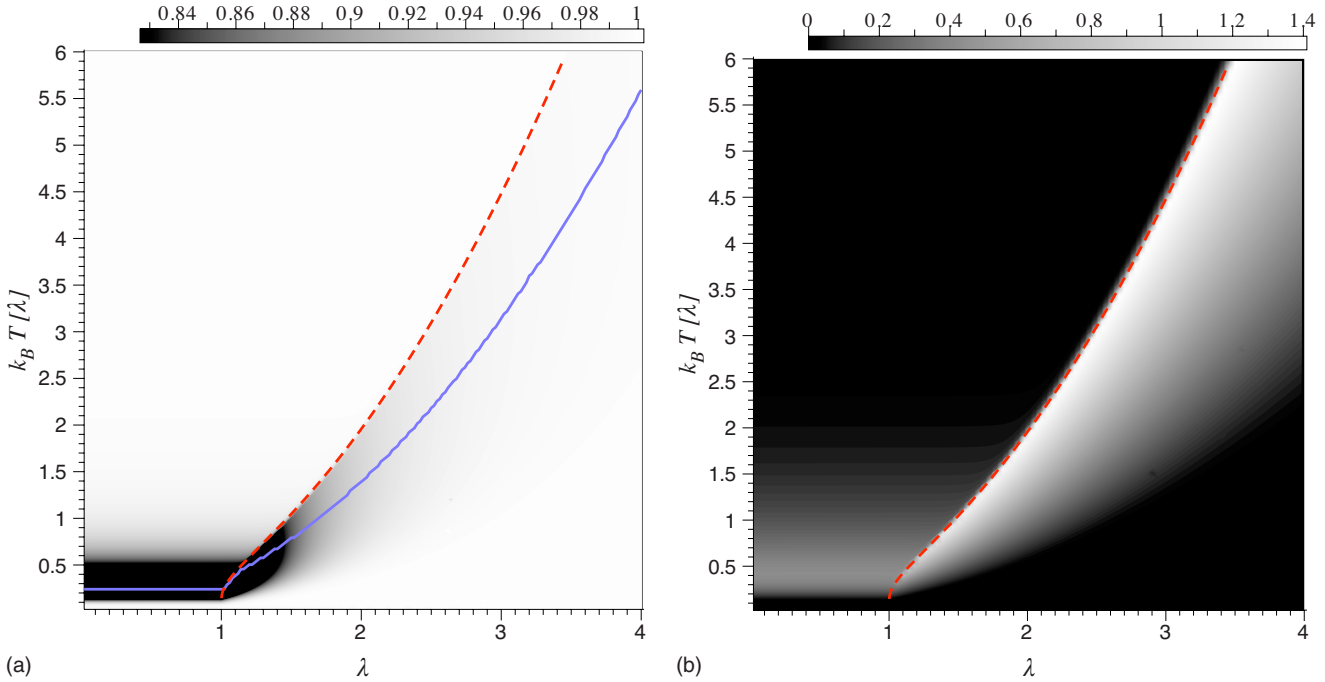


FIG. 3. (Color online) Fidelity (left) and specific heat (right) of the Dicke model for $\omega = \omega_0 = 1$, $N = 10\,000$, $\delta T = 0.001$, and $\delta\lambda = 0$. On the left plot, the minimum of fidelity for fixed λ is indicated with a solid line. The thermal phase transition line (dashed line in both plots) in the superradiant phase ($\lambda > 1$) is indicated by a discontinuity in specific heat and, accordingly, also in fidelity. The decay of fidelity in the normal phase ($0 < \lambda < 1$) is due to a crossover instead of a thermal phase transition. The jump instead of a divergence in the specific heat indicates that the thermal phase transition in Dicke model belongs to a type-B second-order phase transition.

fluctuations tend to wash out the information about phase transitions encoded in the fidelity, an effect we will discuss in more detail in Sec. IV.

B. Type B: discontinuity of second-order derivatives of free energy

A common type of transitions is characterized by a discontinuity or jump of second order derivatives of the free energy at the critical point. This is the case, for instance, in systems described by a simple Landau-Ginzburg theory [21]. In such systems fidelity will not present in general a minimum at the critical points, but somewhere else in the phase diagram. A good example of these type of transitions is the Dicke model, a collection of N two-level atoms interacting with a single bosonic mode via a dipole interaction with an atom-field coupling strength λ [23]. The Hamiltonian of the Dicke model can be written as

$$H = \omega \left[\frac{\omega_0}{\omega} J_z + a^\dagger a + \frac{\lambda}{\sqrt{N}} (a^\dagger + a)(J_+ + J_-) \right], \quad (11)$$

where a and a^\dagger are annihilation and creation operators of the bosonic mode; J_z , J_+ , and J_- are angular momentum operators of the total spin of the system; ω and ω_0 are the natural boson and spin frequencies of the decoupled system; and λ is the spin-boson interaction strength. The energy scale is determined by ω and ω_0 , and phase transitions are controlled by the controlling parameter λ . The model described by Hamiltonian (11) exhibits both a second-order thermal phase transition [24] and a quantum phase transition [25,26], which

has been studied using ground-state fidelity [9]. Here we will study the phase diagram of the Dicke model at finite temperatures using mixed-state fidelity (4). The exact partition function of the Dicke model under the rotating wave approximation (RWA) is [26]

$$Z = 2 \int_0^\infty dr r e^{-\beta r^2} \left[2 \cosh \left(\frac{\beta \omega_0}{2} \sqrt{1 + \frac{4\lambda^2 r^2 \omega^2}{N\omega_0^2}} \right) \right]^N. \quad (12)$$

From this partition function one can obtain that there is a second-order phase transition for $\lambda \geq 1$ at a critical temperature [25,26]

$$\frac{1}{k_B T_c} = \frac{2}{\omega_0} \tanh^{-1} \left(\frac{\omega_0}{\omega \lambda^2} \right). \quad (13)$$

From the partition function of Eq. (12), we obtain the fidelity and the specific heat of the Dicke model (see in Fig. 3 the case of $\omega = \omega_0 = 1$, $\delta T = 0.001$, and $\delta\lambda = 0$).

There are three aspects to highlight from the fidelity and specific heat shown in Fig. 3. First, in the region where there is a thermal phase transition, $\lambda \geq 1$, the minimum of fidelity does not coincide with the phase boundary line. This is easily attributable to the absence of a divergence in the specific heat, which by means of Eq. (5) implies that the minimum of fidelity need not be correlated to the transition line. Second, fidelity presents minima in the region $0 < \lambda < 1$, where the system only has a crossover [as seen from the specific heat, Fig. 3(b)]. This is again explained by the relation between fidelity and specific heat, Eq. (5): all maxima of the specific

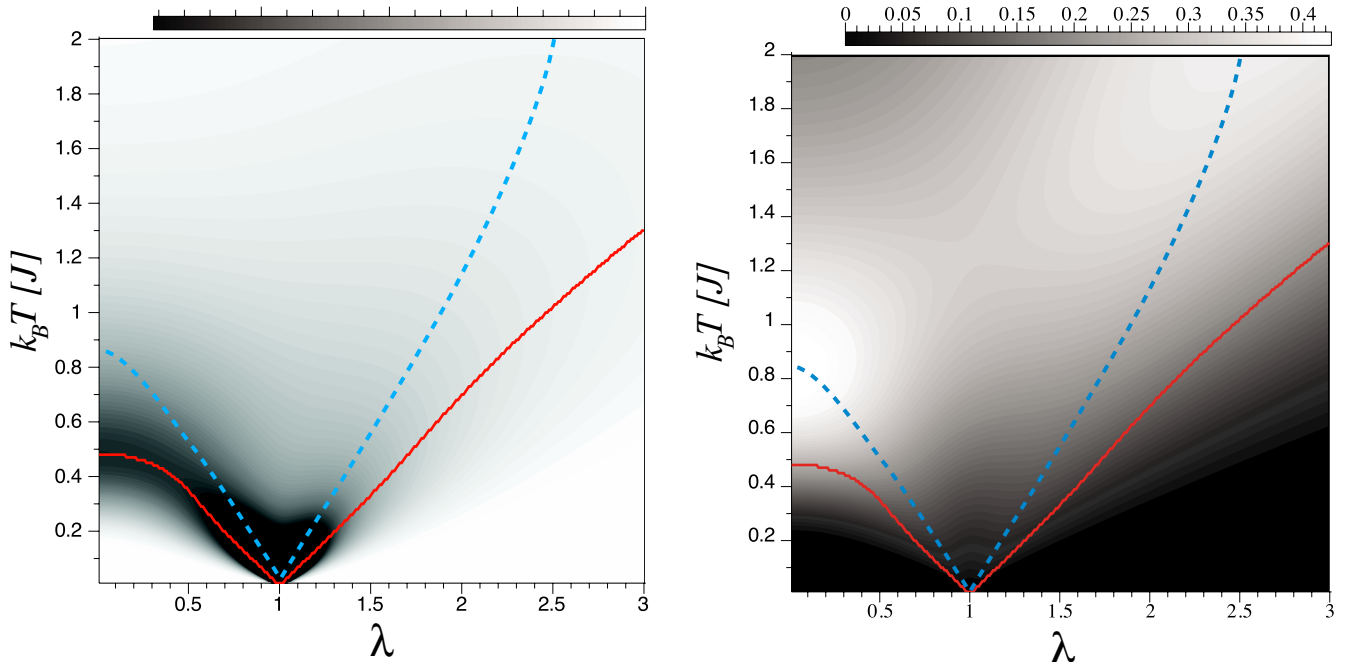


FIG. 4. (Color online) Fidelity $\mathcal{F}_\beta(\beta_0, \beta_1, \lambda)$ (left) and specific heat (right) of 1D transverse Ising model with coupling J in the λ - T plane. The solid line indicates the minimum of fidelity, while the dashed line shows the maximum of the specific heat. Here, the total spin number is $N=10\,000$, $\delta T=0.001$, and $\delta\lambda=0$.

heat (which may not necessarily imply a thermal phase transition) will become minima of the fidelity. We will explore more of this point in the next section. Third, even though the specific heat has a visible discontinuity at the critical points, fidelity changes rather continuously across the phase boundary, especially at high temperatures. Here we find a surprise, since from Eq. (5) we would expect fidelity to be discontinuous at the critical points too. However, as mentioned before, thermal fluctuations affect fidelity strongly, and this discontinuity is washed out for high temperatures. With these three observations combined, we see that the usual fidelity approach is actually not good to distinguish criticality in type-B phase transitions: it cannot correctly signal the critical points with its minima, and is not reliable with discontinuities. Furthermore, as in the $0 < \lambda < 1$ region of the Dicke model, fidelity might identify simple crossovers as phase transitions. In the following section we will study at depth more these problems and possible solutions.

IV. CROSSOVERS AND THERMAL FLUCTUATIONS

As discussed in the Introduction, geometrical arguments about fidelity in critical systems lead us to expect that fidelity will have a minimum at the critical transition points. We just saw that this should be extended at least to identify discontinuities in fidelity with type-B phase transition points (akin to the behavior of ground state fidelity in first-order QPTs). In this section we explore the following question: is it possible to use fidelity, a quantum information tool, to fully characterize a critical system at nonzero temperature, i.e., by properly identifying all transition points of the phase diagram?

A. Crossovers vs thermal phase transitions

The free energy of a system is analytic everywhere in the λ - T plane except at phase transition points. But, there are many “normal” systems without transitions, i.e., where free energy is analytic simply everywhere. Nevertheless, this does not exclude the possibility that at some points the specific heat can become very large, e.g., at the so-called crossover points [1]. In fact, type-A transitions in finite systems look similar to crossovers that become divergences only at the thermodynamic limit. Because of the relation between fidelity and specific heat, Eq. (5), we expect that fidelity will also have a minimum at the crossover point. This, in principle, can be seen as another feature of fidelity, i.e., that fidelity can also be used to characterize crossovers [18]. However, we are interested in the different problem of detecting a phase transition using fidelity.

Let us consider the example of the 1D transverse Ising model (TIM) with Hamiltonian $H = -J \sum_{i=1}^N (\sigma_i^z \sigma_{i+1}^z + \lambda \sigma_i^x)$. The partition function of the system is [27]

$$Z = 2^N \exp \left\{ \frac{N}{\pi} \int_0^\pi dk \ln \left[\cosh \left(\frac{2J \sqrt{1 + \lambda^2 - 2\lambda \cos k}}{2k_B T} \right) \right] \right\}. \quad (14)$$

We show a contour plot of fidelity for the 1D TIM in Fig. 4 for $\delta T=0.001$ and $\delta\lambda=0$ (a similar figure can be found in Ref. [16]). In this figure we see a minimum of fidelity following what seems to be a phase transition line. We know, however, that this model does not have phase transitions for finite temperature (one way to see this is to map the 1D TIM into a classical 2D Ising model, where the inverse temperature is the effective finite size in the extra dimension of the

classical system). Thus, with only this information fidelity alone may not be able to distinguish simple crossovers from proper thermal phase transitions. For example, a simple fidelity approach would have led us to postulate a thermal phase transition for the Dicke model for $0 \leq \lambda < 1$ (see Fig. 3), which we know does not exist from the exact solution. In order to make this distinction, we must resort to traditional statistical mechanics criteria—such as the free energy and its derivatives. We show in Fig. 4 the specific heat for the 1D TIM in the λ - T plane, which clearly does not have a divergence or a discontinuity. In addition, the “crossover line” found with the minimum of fidelity deviates slightly from the “crossover line” $T_c \sim |1 - \lambda|$ obtained from maximum of specific heat (see Fig. 4) and magnetic susceptibility [28]. The later agrees well with results obtained from fidelity susceptibility and other discussions [29,30].

We identify then two difficulties for fidelity to detect a crossover line: First, that it is indistinguishable from the behavior of fidelity at a critical point and second, that it misses the position of the correct crossover line. To solve the first problem—and as is common in statistical mechanics calculations—we can consider the finite-size scaling of fidelity. Indeed, at a proper thermal phase transition specific heat and other thermodynamical quantities (and therefore fidelity) will show a very different behavior with system size when compared to a crossover. This approach, however, could be limited to systems where divergences develop fast enough with system size—for example, a logarithmic divergence might require extensive numerical power to be observed. On the other hand, such systems are difficult to study also with traditional quantities, and therefore fidelity remains as good an indicator of criticality as any.

The solution to the second problem is simpler but more subtle: by choosing a perturbation that is proportional to temperature $\delta T \sim T$, fidelity correctly signals the crossover line. This is because with a fixed perturbation in temperature fidelity is not simply related to specific heat but it has an extra dependence with T [see Eq. (5)]. The same dependence of the perturbation on fidelity will be discussed in the next subsection as a way to reduce the effect of thermal fluctuations on fidelity.

B. Fidelity and thermal fluctuations

With fidelity arising from a quantum information approach, it is natural to question its behavior for moderate to high temperatures, where quantum effects—such as noncommutation of operators—might be obscured. Indeed, thermal fluctuations can wash out all information about phase transitions characterized by ground-state fidelity [20]. We already saw in the Dicke model of previous sections that fidelity singularities become blurred for high temperatures, while the specific heat shows a singularity for all temperatures. We refer again to Fig. 3 for comparisons between \mathcal{F} and C_v . We see that the minimum of fidelity (or its discontinuity) becomes increasingly less prominent for higher temperatures, eventually disappearing from the numerical precision. On the contrary, specific heat is not influenced by thermal fluctuations and is a robust indicator of criticality up to very high temperatures.

Let us give a heuristic analysis of the influence of thermal fluctuations on mixed-state fidelity. The perturbation in temperature δT can be expressed as

$$\delta\beta = \frac{1}{T} - \frac{1}{T + \delta T} = \frac{\delta T}{T(T + \delta T)}. \quad (15)$$

Hence, from Eq. (5) we can write fidelity as

$$\mathcal{F}_\beta \approx e^{-[(\delta T)^2/8T^2]C_v}. \quad (16)$$

From this equation we can see that when temperature increases, for a fixed energy scale and fixed δT , the effect on fidelity of the singularity of specific heat C_v at critical points will be attenuated. It is important to highlight that the fidelity susceptibility [18] $\chi_\beta = C_v/(4\beta^2) = T^2 C_v/4$ will not be affected by thermal fluctuations at high temperature. Hence, even though fidelity itself may not be a good indicator of thermal phase transitions at high temperature, fidelity susceptibilities seem to be robust—although this is just because they are proportional to traditional quantities such as specific heat and susceptibility.

Equation (16) points to a possible workaround to this high-temperature problem. Indeed, if we choose a perturbation δT that increases with temperature then we can obtain a fidelity \mathcal{F}_β that remains insensitive to temperature fluctuations. For example, if $\delta T = \alpha T$, such that $T_1 = (1 + \alpha)T_0$, then the minimum of fidelity depends exclusively on the specific heat and not directly on temperature. The choice of a parameter-dependent perturbation seems a simple one, but we remark that it is unusual in fidelity studies in general, where fixed perturbations are the norm. The reason why it is necessary in our case is that in this way the perturbation is always larger than the energy scale set by the temperature fluctuations. From Eq. (7) we see that we should also consider a field perturbation that depends on temperature, although with a different law.

V. FIDELITY IN THE LIPKIN-MESHKOV-GLICK MODEL—A CASE STUDY

For all the limitations we have discussed, fidelity decay or jump at the critical points is still a necessary condition for a phase transition to exist. Therefore, in the cases where fidelity is easier to compute than traditional observables from statistical mechanics—such as magnetic susceptibility and specific heat—it can certainly be used as a precriterion to explore the phase diagram of a system for potential phase transitions. In order to test the predictive power of fidelity for thermal phase transitions, we used it to study the phase diagram of the Lipkin-Meshkov-Glick (LMG) [31] model of N globally coupled spins with an external magnetic field. The Hamiltonian of the LMG model in units of the coupling energy is

$$H = -\frac{1}{N} \sum_{i < j} (\sigma_i^x \sigma_j^x + \gamma \sigma_i^y \sigma_j^y) - \lambda \sum_i \sigma_i^z, \quad (17)$$

where σ_i^α , $\alpha = x, y, z$ are the Pauli matrices of the i th spin, γ is an anisotropy parameter, and λ is an applied external field.

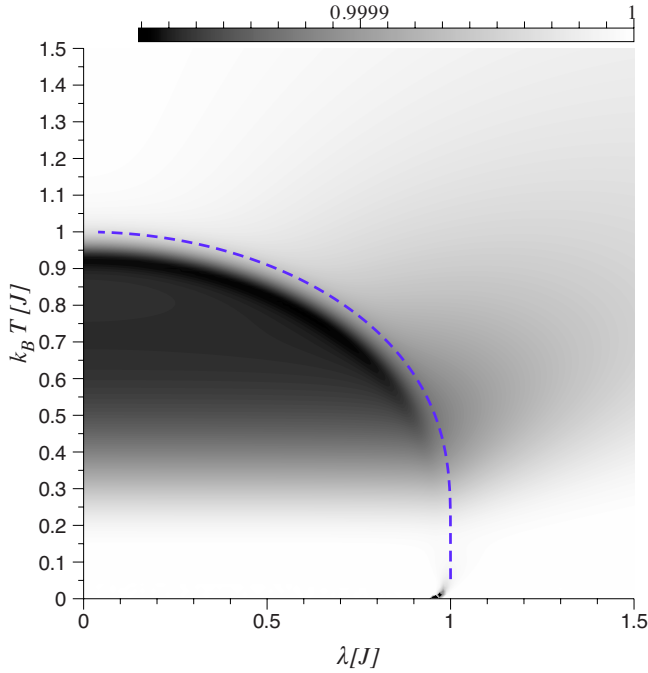


FIG. 5. (Color online) Temperature fidelity of LMG model for $N=800$, $\delta T=0.001$, and $\gamma=0.2$. Both the thermal phase transitions $T_C=\lambda/\tanh^{-1}\lambda$ ($0\leq\lambda\leq 1$) and quantum phase transition at $\lambda=1$, $T=0$ are indicated by the discontinuity and decay of fidelity, respectively. Nevertheless, for the thermal phase transition, the discontinuity of fidelity deviates slightly from the phase boundary given by the mean-field result (dashed line), although this is still within the deviation expected for a finite size system.

QPT of this model at $T=0$, $\lambda=1$ has been extensively studied [32]. However, as far as we know, the nonzero phase diagram of this model has not been explored before. In the following we will systematically study the finite-temperature thermal phase transition of this system. We approached this problem without previous knowledge of its phase diagram, partly to test the usefulness of fidelity, and partly (to be honest) out of ignorance. In order to solve this model numerically we used a large spin $S=N/2$ representation

$$H = -\frac{1+\gamma}{N}\left(\vec{J}^2 - J_z^2 - \frac{N}{2}\right) - 2\lambda J_z - \frac{1-\gamma}{2N}(J_+^2 + J_-^2), \quad (18)$$

where $J_\alpha = \sum_{i=1}^N \sigma_i^\alpha / 2$, $\alpha=x,y,z$ is the total angular momentum operator. This is convenient because Hamiltonian (18) does not mix subspaces with different projection of the angular momentum, and one just has to diagonalize matrices of size $N \times N$.

Indeed, our fidelity studies detected something that appeared to be a thermal phase transition in the λ - T diagram (the anisotropy parameter γ turns out to be not very important as we will see shortly), see Fig. 5. Here we choose $\delta T=0.001$ and $\delta\lambda=0$. We confirmed the existence of a thermal phase transition with further numerical calculations of the specific heat and susceptibility, shown in Fig. 6, and by a mean field calculation that we present here (we are not aware of such a calculation for finite temperature in the literature).

Adding and subtracting the magnetization along the $\alpha=x,y$ direction, $M_\alpha = \frac{1}{N}\langle \sum_{i=1}^N \sigma_i^\alpha \rangle$, the LMG Hamiltonian (17) can be written as

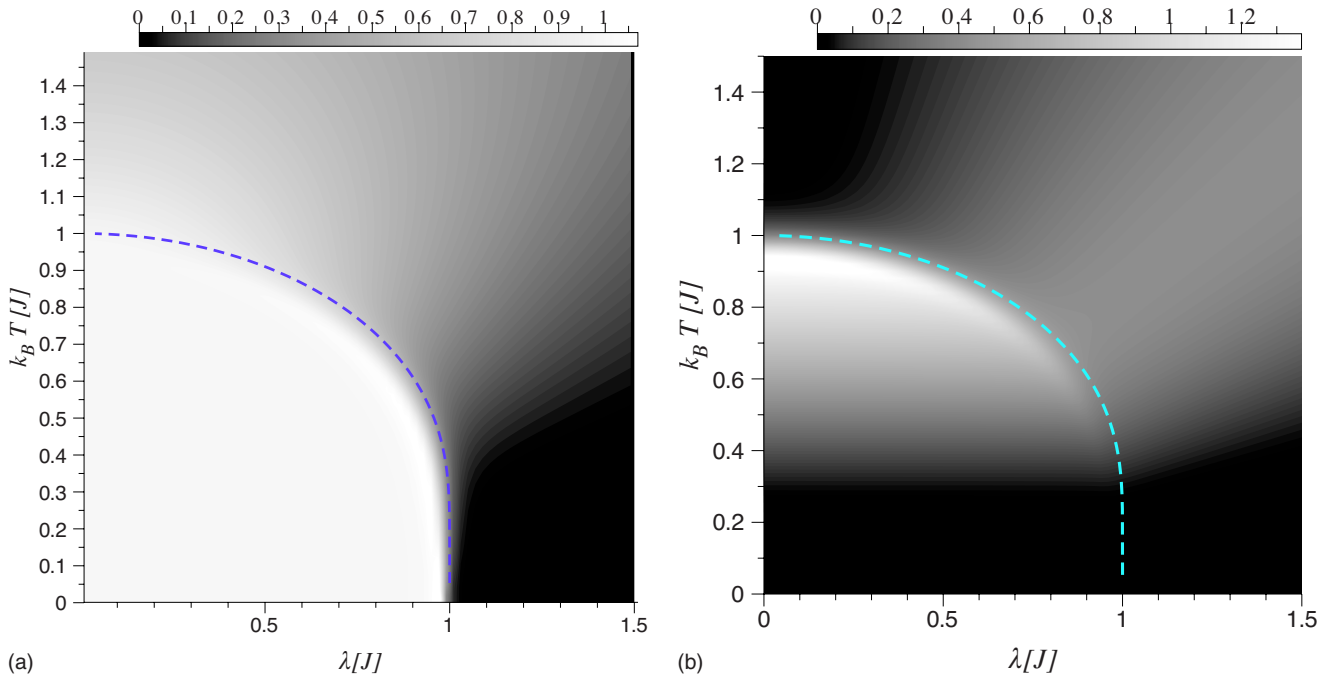


FIG. 6. (Color online) (left) Magnetic susceptibility χ and (right) specific heat C_V of the LMG model for $N=800$, $\gamma=0.2$. The phase boundary given by specific heat and susceptibility agrees well with that of mean-field result (shown in dashed line). Notice however that the discontinuity in χ for small λ is less pronounced, given that the phase boundary lies at almost constant temperature (the reverse happens for the specific heat C_V at low temperatures and $\lambda \approx 1$).

$$\begin{aligned}
H = & -\frac{1}{2N} \sum_{i,j} [(\sigma_i^x - M_x)(\sigma_j^x - M_x) + M_x(\sigma_i^x + \sigma_j^x) \\
& + \gamma(\sigma_i^y - M_y)(\sigma_j^y - M_y) + \gamma M_y(\sigma_i^y + \sigma_j^y) - M_x^2 - \gamma M_y^2] \\
& + \frac{1+\gamma}{2} - \lambda \sum_i \sigma_i^z. \quad (19)
\end{aligned}$$

We will see that M_α is also the order parameter of the phase transition of LMG model, in analogy with the 1D quantum XY model. Using a mean-field approximation, the quadratic terms cancel out, and the Hamiltonian (19) is reduced to

$$\begin{aligned}
H = & -\sum_{i=1}^N \left(M_x \sigma_i^x + \gamma M_y \sigma_i^y + \lambda \sigma_i^z - \frac{1}{2} M_x^2 - \frac{\gamma}{2} M_y^2 - \frac{1+\gamma}{2N} \right) \\
\approx & -\sum_{i=1}^N \left(M_x \sigma_i^x + \gamma M_y \sigma_i^y + \lambda \sigma_i^z - \frac{1}{2} M_x^2 - \frac{\gamma}{2} M_y^2 \right), \quad (20)
\end{aligned}$$

where we have ignored the last term because this term is vanishingly small in comparison with other terms in the thermodynamics limit. The mean-field Hamiltonian is a sum of decoupled single-spin Hamiltonians that can be diagonalized directly, with eigenenergies

$$\mathcal{E}_\pm \approx \pm \sqrt{M_x^2 + \gamma^2 M_y^2 + \lambda^2} + \frac{1}{2}(M_x^2 + \gamma^2 M_y^2) \quad (21)$$

and their corresponding eigenstates

$$\begin{aligned}
|\mathcal{E}_+\rangle &= \frac{(M_x - i\gamma M_y)|\uparrow\rangle + (\mathcal{E}_+ - \lambda)|\downarrow\rangle}{\sqrt{(M_x^2 + \gamma^2 M_y^2) + (\mathcal{E}_+ - \lambda)^2}}, \\
|\mathcal{E}_-\rangle &= \frac{(M_x - i\gamma M_y)|\uparrow\rangle + (\mathcal{E}_- - \lambda)|\downarrow\rangle}{\sqrt{(M_x^2 + \gamma^2 M_y^2) + (\mathcal{E}_- - \lambda)^2}}, \quad (22)
\end{aligned}$$

where $|\uparrow\rangle$ and $|\downarrow\rangle$ are eigenstates of σ^z . The self-consistent equations for the magnetization (order parameter) are

$$\begin{aligned}
M_x = \langle \sigma_i^x \rangle &= \frac{1}{z} e^{-\beta \mathcal{E}_+} \langle \mathcal{E}_+ | \sigma_i^x | \mathcal{E}_+ \rangle + \frac{1}{z} e^{-\beta \mathcal{E}_-} \langle \mathcal{E}_- | \sigma_i^x | \mathcal{E}_- \rangle, \\
M_y = \langle \sigma_i^y \rangle &= \frac{1}{z} e^{-\beta \mathcal{E}_+} \langle \mathcal{E}_+ | \sigma_i^y | \mathcal{E}_+ \rangle + \frac{1}{z} e^{-\beta \mathcal{E}_-} \langle \mathcal{E}_- | \sigma_i^y | \mathcal{E}_- \rangle, \quad (23)
\end{aligned}$$

where $z = e^{-\beta \mathcal{E}_+} + e^{-\beta \mathcal{E}_-}$ is the partition function of the mean-field single-spin Hamiltonian. Combining Eqs. (21)–(23) we obtain the following two self-consistent equations:

$$\begin{aligned}
M_x &= \frac{\tanh[\beta \sqrt{\lambda^2 + M_x^2 + \gamma^2 M_y^2}]}{\sqrt{\lambda^2 + M_x^2 + \gamma^2 M_y^2}} \times M_x, \\
M_y &= \frac{\tanh[\beta \sqrt{\lambda^2 + M_x^2 + \gamma^2 M_y^2}]}{\sqrt{\lambda^2 + M_x^2 + \gamma^2 M_y^2}} \times \gamma M_y. \quad (24)
\end{aligned}$$

For $\gamma \neq 1$, the above two equations have nontrivial solutions only when either $M_x = 0$ or $M_y = 0$. The two parameters can be further determined by the condition of minimum free energy.

At absolute zero, the free energy equals the ground-state energy \mathcal{E}_- . It is not difficult to find that when $\gamma < 1$, $M_x \neq 0$, $M_y = 0$ leads to the minimum ground-state energy, while when $\gamma > 1$, $M_x = 0$, $M_y \neq 0$ leads to the minimum energy (and $M_x = M_y$ for $\gamma = 1$). For example, when $\gamma < 1$, the self-consistent equation is reduced to

$$T = \frac{\sqrt{M_x^2 + \lambda^2}}{\tanh^{-1} \sqrt{M_x^2 + \lambda^2}}. \quad (25)$$

In the λ - T plane the phase boundary can be determined by setting the order parameter to be zero $M_x = 0$. Then, the critical temperature as a function of external magnetic field λ is

$$T_c = \frac{\lambda}{\tanh^{-1} \lambda}, \quad 0 \leq \lambda \leq 1. \quad (26)$$

This mean-field result agrees well with the phase boundary obtained by fidelity (Fig. 5) and traditional criteria, such as specific heat C_v and magnetic susceptibility χ (see Fig. 6), because the coordination number of the LMG model is $N - 1$, i.e., it is big enough to ensure the mean-field approximation is reliable.

Thus, we have detected a phase transition with fidelity, which we then confirmed through magnetic susceptibility and specific heat. Both results agree with the analytical result from mean-field theory. To the best of our knowledge, these events occur in this order, and lends support to our discussion above that fidelity is a good precriterion for testing phase boundaries.

VI. DISCUSSION AND CONCLUSIONS

In the above Sec. III through Sec. V, we discussed the applicability of \mathcal{F}_β to characterize thermal phase transitions, and indicated some of its limitations. Here we would like to further consider the applications of \mathcal{F}_λ and the “quantum” (zero temperature) to “classical” (nonzero temperature) transition of the system [1,33]. For high temperatures, statistical fluctuations dwarf quantum ones, and the importance of uncertainty relations for the approximation in Eq. (6) decreases. In this case, the fidelity becomes a function of χ and the phase transition is classical [1,33]. This means that with the increase of temperature, the fidelity criteria \mathcal{F}_λ for QPT becomes equivalent to the susceptibility criteria for thermal phase transitions. Nevertheless, at low temperature, especially at zero temperature, the two criteria \mathcal{F}_λ and χ differ drastically due to the quantum and classical nature of the phase transitions. Thus, one can say that the “quantum” fidelity susceptibility χ_λ is different from the classical susceptibility χ only at low temperatures, and especially at zero temperature. This heuristic analysis agrees well with the result of Refs. [1,33], that with the increase of the temperature the phase transition changes from “quantum” to “classical.”

In summary, fidelity is a good tool to investigate quantum phase transitions, and has been extensively studied. However, when extending to finite-temperature thermal phase transition, we should be careful about the following subtle aspects. (1) Fidelity decay occurs at both thermal phase transitions points and crossover lines, thus we cannot rely on

fidelity decay alone as an indication of phase transition. For this, we must fall back on traditional criteria such as the free energy and its derivatives, or fidelity susceptibility, or the finite-size scaling of fidelity. (2) For second-order phase transitions with a divergence in second derivatives of free energy (type A), drastic fidelity decay only occurs at critical points, and critical lines can be reliably identified. However, for type-B transition—with a discontinuity instead of a divergence—fidelity decay occurs at many places besides critical points, and maximum decay of fidelity may not correspond to phase transition points. Fidelity itself might show a discontinuity, but it might be visible only for low temperatures. Hence, the standard fidelity criterion for second-order thermal phase transitions is more applicable to type-A than to type-B thermal phase transitions. (3) In general, the fidelity approach seems more applicable to low-temperature thermal phase transitions only. For a fixed energy scale and a fixed δT , when the critical temperature is very high, fidelity may fail to signal the transition because thermal fluctuations wash out all the relevant information encoded in fidelity. In comparison, fidelity susceptibility and traditional criteria based on free energy are not affected by thermal fluctuations and are good for any temperature. A solution to this problem is to use a perturbation that depends on temperature. Our calculations suggest that it would be sufficient to use $\delta T \sim T$ and $\delta \lambda \sim \sqrt{T}$ to keep the sensitivity of fidelity intact with temperature. We also showed that with this simple but nontrivial choice of perturbation, fidelity can signal correctly the position of crossover lines.

Before concluding this paper, we would like to point out that, despite its limitations for finite-temperature transitions, fidelity can still be a very useful precriterion to detect thermal phase transitions, especially in systems where we have no prior knowledge about its order parameter and symmetries, or even topological thermal phase transitions without an order parameter and symmetry breaking. Because of its simple form, we can plot the fidelity of the system and then exclude the possibility of thermal phase transitions regimes without fidelity singularities. Afterwards, we can focus on suspect areas using free energy and traditional criteria or fidelity susceptibility or finite-size scaling analysis of fidelity to distinguish crossovers from thermal phase transitions.

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APPENDIX A: SPECIFIC HEAT AND MIXED-STATE FIDELITY

We will see here the relation between fidelity with a temperature perturbation and specific heat. From the standard definition $C_v = -T \partial^2 F / \partial T^2$, where F is the free energy, and for a sufficiently small perturbation $\delta T / T \ll 1$, we can approximate

$$\begin{aligned} C_v(T) &\simeq -T \left[\frac{F(T + \delta T/2) + F(T - \delta T/2) - 2F(T)}{(\delta T/2)^2} \right] \\ &\simeq -\frac{2T^2}{(\delta T/2)^2} \ln \frac{Z(T)}{\sqrt{Z(T + \delta T/2)Z(T - \delta T/2)}} \\ &\quad + \frac{2T}{\delta T} \ln \frac{Z(T + \delta T/2)}{Z(T - \delta T/2)}, \end{aligned} \quad (\text{A1})$$

where we have used $F = -T \ln Z(T)$. Now, multiplying by $\delta \beta^2 / \beta^2 = \delta T^2 / (T + \delta T)^2$, and keeping the lowest order terms in $\delta T / T$,

$$-\frac{(\delta \beta)^2}{8\beta^2} C_v \simeq \ln \frac{Z\left(\frac{\beta_0 + \beta_1}{2}\right)}{\sqrt{Z(\beta_0)Z(\beta_1)}}, \quad (\text{A2})$$

where $\beta_0 = 1/(T_0 - \delta T/2)$, and $\beta_1 = 1/(T_0 + \delta T/2)$. We thus obtain the relation between temperature fidelity \mathcal{F}_β and specific heat

$$\mathcal{F}_\beta(\beta_0, \beta_1, \lambda) = \frac{Z\left(\frac{\beta_0 + \beta_1}{2}\right)}{\sqrt{Z(\beta_0)Z(\beta_1)}} \simeq e^{-[(\delta \beta)^2 / 8\beta^2] C_v}. \quad (\text{A3})$$

APPENDIX B: NONCOMMUTATIVE DENSITY MATRIX

We look for a simplification of the perturbation in field fidelity

$$\mathcal{F}_\lambda(\beta, \lambda_0, \lambda_1) = \text{Tr} \sqrt{\sqrt{\rho_0} \rho_1 \sqrt{\rho_0}}, \quad (\text{B1})$$

where $\rho_\alpha = \exp[-\beta H(\lambda_\alpha)] / Z$. Usually, $H(\lambda_0)$ and $H(\lambda_1)$ do not commute with each other. However, we can use the Trotter-Suzuki formula [34] to approximate

$$\begin{aligned} &\left\| \sqrt{\rho_0} \rho_1 \sqrt{\rho_0} - \frac{e^{-\beta(H(\lambda_0) + \beta H(\lambda_1))}}{Z(\beta, \lambda_0)Z(\beta, \lambda_1)} \right\| \\ &< \beta^3 \Delta_2[H(\lambda_0), H(\lambda_1)] e^{\beta \|H(\lambda_0)\| + \beta \|H(\lambda_1)\|}, \end{aligned} \quad (\text{B2})$$

where

$$\begin{aligned} \Delta_2[H(\lambda_0), H(\lambda_1)] &= \frac{1}{12} \left(\left\| [[H(\lambda_0), H(\lambda_1)], H(\lambda_1)] \right\| \right. \\ &\quad \left. + \frac{1}{2} \left\| [[H(\lambda_0), H(\lambda_1)], H(\lambda_0)] \right\| \right). \end{aligned} \quad (\text{B3})$$

Thus, we have

$$\begin{aligned} \mathcal{F}_\lambda(\beta, \lambda_0, \lambda_1) &\simeq \frac{Z\left(\beta, \frac{\lambda_0 + \lambda_1}{2}\right)}{\sqrt{Z(\beta, \lambda_0)Z(\beta, \lambda_1)}} \\ &\simeq \frac{Z(\beta, \lambda_0)}{\sqrt{Z\left(\beta, \lambda_0 + \frac{\delta \lambda}{2}\right)Z\left(\beta, \lambda_0 - \frac{\delta \lambda}{2}\right)}} \end{aligned} \quad (\text{B4})$$

which is Eq. (6). The validity condition (B2) indicates that at

high temperature or small perturbation (typically $\beta^3 \delta\lambda^3 \ll 1$), the fidelity criteria \mathcal{F}_λ for QPT becomes equivalent to susceptibility criteria for thermal phase transition and thus the phase transition changes from “quantum” to “classical.”

APPENDIX C: MAGNETIC SUSCEPTIBILITY AND MIXED-STATE FIDELITY

Similar to Appendix A, we approximate the magnetic susceptibility

$$\chi = -\frac{\partial^2 F}{\partial \lambda^2} \approx \frac{F\left(\lambda_0 + \frac{\delta\lambda}{2}\right) + F\left(\lambda_0 - \frac{\delta\lambda}{2}\right) - 2F(\lambda_0)}{(\delta\lambda/2)^2}. \quad (\text{C1})$$

Hence we have

$$\begin{aligned} -\frac{\beta(\delta\lambda)^2}{8}\chi &\approx -\frac{(\delta\lambda)^2}{8T} \frac{F\left(\lambda_0 + \frac{\delta\lambda}{2}\right) + F\left(\lambda_0 - \frac{\delta\lambda}{2}\right) - 2F(\lambda_0)}{(\delta\lambda/2)^2} \\ &\approx \frac{2 \ln Z(\lambda_0) - \ln Z\left(\lambda_0 + \frac{\delta\lambda}{2}\right) - \ln Z\left(\lambda_0 - \frac{\delta\lambda}{2}\right)}{2} \\ &\approx \ln \frac{Z(\lambda_0)}{\sqrt{Z(\lambda_0 + \delta\lambda/2)Z(\lambda_0 - \delta\lambda/2)}}. \end{aligned} \quad (\text{C2})$$

From Appendix B, we obtain Eq. (7)

$$\mathcal{F}_\lambda(\beta, \lambda_0, \lambda_1) \approx \frac{Z(\lambda_0)}{\sqrt{Z\left(\lambda_0 + \frac{\delta\lambda}{2}\right)Z\left(\lambda_0 - \frac{\delta\lambda}{2}\right)}} \approx e^{-[\beta(\delta\lambda)^2/8]\chi}. \quad (\text{C3})$$

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